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The View from HQ

by Dimitri Kusnezov

I have been spending much of my time these days thinking about science, technology and engineering and the role of the laboratories and how that will be reflected in the Complex of the future. This is on my mind for two reasons: one is my responsibility to produce a science and technology roadmap for Complex 2030—Defense Program's vision for what we should be doing in 2030—and how we plan to get there. The second reason is to determine what this means for the near-term roles of the laboratories. For some time now I have been concerned that too much of our national security mission is tied to the nuclear weapons monolith, leveraged on the continuation of an enterprise that has not fully transitioned out of the cold-war. Today's and tomorrow's threats are far different than what we worried about decades ago, but our mission space has never been redefined to meet our new reality. While the laboratories have recognized some of this, the question here is whether there is a mission space that requires federal land-lording and strategic investment that we are not planning for today. I believe this is the case, and in conjunction with the Complex 2030 roadmap, I am endeavoring to push this along.

Is Complex 2030 enough for planning for science and technology? That depends on whether it is largely focused within the weapons' account. We need to think about investments that might currently fit in our mission space, but which might be better suited to tomorrow's threats. With such ponderings, combined with events during the last two years, it has been a wild ride. Both Los Alamos and Lawrence Livermore are under new ownership; NNSA has experienced leadership changes at all levels; and the RRW decision has spawned not only public debate, but perhaps an uncommon level of inter-lab public discourse, and is now the subject of congressional language that has taken both sides of the issue. Things could not be murkier. But all this indicates to me that we are at a cross-road, and with this turmoil comes opportunity for change.

So what does this have to do with ASC? We are faced with quite a few challenges. First, in the near term, we will be facing the challenge of reducing the footprint of where we site our largest platforms in the 2010 horizon. This does not mean that only host sites can field platforms, but rather where we actually locate the most costly investments. It is entirely possible that the intellectual development of new technologies is not co-located with the final production system. We will continue to work with the ASC Execs to better understand this issue during 2008. It is entirely possible as well that Congressional direction will decide our hand one way or another. Second, in the area of codes, we are not anywhere near achieving predictive capability yet. We are pioneering computational science at the most remarkable scales, and together we are learning how to define notions of predictivity through verification, validation and uncertainty quantification. We are uncovering the challenges that the rest of the world will eventually face, and this gives us the chance to define this frontier in a manner that can have a lasting impact. The modeling efforts at the laboratories are crucial for success, in terms of both development and implementation. Further progress of the thermonuclear burn initiative in FY2007 and 2008 is an important part of this.

To me, ASC remains the focal point through which we enable not only stewardship, as the only conduit to conduct nuclear tests (albeit virtually), but as an exemplar of the future of national security sciences. It is indeed an exciting time.

ASC Program Begins Work on National Code Strategy

The ASC Program has embarked on developing a national code strategy designed to help achieve the Program's goal of delivering a credible and sustainable predictive simulation capability for stockpile stewardship. This code strategy is one of the next major programmatic plans being developed by the tri-lab ASC community and Headquarters. The strategy will be a high-level "design document" for the future code development activities sponsored by ASC, and it complements the larger *ASC Roadmap* and the Predictive Capability Framework, directed at how we implement the program through our code portfolio and supporting research.

A team of three representatives each from Sandia, Los Alamos, and Lawrence Livermore national laboratories, plus representatives from NNSA Headquarters, completed its first meeting on May 1 and 2, 2007, at Sandia. A wide range of topics was discussed, including an overview of current capabilities, how code and method diversity impact the ability to support stockpile stewardship, and the potential impact of coming changes in computational technologies on the code portfolio.

The near-term goal is to begin developing a vision for ASC's Integrated Codes program element as it would exist in 2018, and to test that vision against a number of possible future scenarios for the larger Stockpile Stewardship Program and Complex 2030. The team will meet again in June to work on these near-term goals. It expects to complete the full strategy in early 2008.

Report of the Predictive Science Panel Issued: Many Examples of Outstanding and World-Class Science

The 2006–2007 Report of the Predictive Science Panel (PSP) noted "many examples of outstanding and world-class science, ranging from awarding-winning materials science simulations and ASC-informed re-analyses of UGT [underground test] data to very high strain-rate materials strength experiments." The PSP meets annually at both Lawrence Livermore (LLNL) and Los Alamos national laboratories to evaluate progress toward the goal of a credible predictive capability, answering the question: How do you know it's right?

LLNL Associate Director for Defense and Nuclear Technologies Bruce Goodwin stated that at the PSP debriefing, the Physics and Engineering Models Program's multi-scale dislocation dynamics work was favorably compared to the groundbreaking work on materials done by Rudolf Peierls in the 1930s. "I'm proud to have our work compared to the seminal work of such a renowned scientist," said Goodwin.

The report also noted, "Progress toward true predictive capability is accelerating, but continuing at the same rate will soon put a strain on both capacity and capability computing assets. At the same time, validating experiments must be adequately supported. Although the science path forward remains clear, this is a critical transitional moment for the ASC Program and for the laboratories' ASC-related efforts. The transition involves expansion of the ASC Program roles to include RRW [the Reliable Replacement Warhead], Complex 2030, and better coordination with supporting experimental science, as well as new petaflop-scale computer acquisitions."

ASC Simulation and V&V Showcased at the ICED-07 Conference, Portugal

François Hemez, of X-1-MV at Los Alamos, was invited to be one of three keynote speakers at the 4th International Conference on Engineering Dynamics (ICED). The ICED is organized by the Instituto Superior Tecnico, Universidade Tecnica de Lisboa. This year, the conference was held in Carvoeiro, Portugal, on April 16–19, 2007. The conference is an international forum where recent advances in the disciplines of testing, modeling, and validation are discussed for engineering applications. One-hundred engineers and scientists attended, originating, for the most part, from Eastern Europe, Western Europe, and the United States. The keynote presentation, entitled "*15 Years of Verifying and Validating Simulations at Los Ala-*

mos" (LA-UR-07-2213), showcased some of the accomplishments of the ASC Program in terms of simulation capability and Verification and Validation (V&V), with an emphasis on engineering applications. The conference web site can be accessed at http://www.dem.ist.utl.pt/~iced2007/.

(Previous page, right) Dr. Nuno Maia, Professor of Mechanical Engineering, Universidade Tecnica de Lisboa, Portugal, and chair of the conference, presenting his opening remarks during the Monday morning plenary session of the 4th ICED.

Red Storm Enters General Availability

Red Storm supercomputer, located at Sandia National Laboratories (Albuquerque, NM) entered the "General Availability" stage on March 26, 2007. This change marked the completion of all initial deployment and testing tasks. The system had been operating in "Limited" availability since September 2005, pending improvements to both the platform and the supporting systems (Red and Black RoSE). The platform upgrades resulted in Red Storm being ranked #2 on the Top 500 list of supercomputers published in November 2006. During General Availability, all new user requests will be honored if the users have legitimate Nuclear Weapons, Directed Stockpile Work, or Alliance partners' project needs.

Current user accounts will remain active.

Sandia welcomes this new stage in Red Storm's activities. The entire Red Storm and Sandia Supercomputing Support teams are looking forward to working with new users to maximize their productivity on the platform.

Critical Decision-0 Approved for ASC Sequoia Supercomputer

The Critical Decision Mission Need Package (CD-0) for the new ASC Sequoia supercomputer was approved and signed on April 23, 2007, by Marty Shoenbauer, acting NNSA Deputy Administrator for Defense Programs. CD-0 approves the NNSA mission need for Sequoia, a new uncertainty quantification (UQ)-focused computer system to be delivered in 2011. The CD-0 package contains a mission need statement, business case, and preliminary project execution plan. It represents the initiation stage of project management activities for Sequoia.

Approval of CD-0 paves the way for the Sequoia project to proceed into definition and execution phases, where the next steps will be to create an industry request for proposal (RFP), evaluation of responses, vendor selection, and contract award. The current Sequoia project schedule calls for approval of Critical Decision 1 (CD-1 Conceptual Baseline Package) and RFP release in September 2007, approval of Critical Decisions 2 and 3 (CD-2/3 Combined Performance Baseline and Construction Readiness Packages) in December 2007, and a contract award early in 2008.

To meet its NNSA and ASC missions, the Sequoia system plans to provide at least 12 times the sustained performance of ASC Purple (sited in 2006) on integrated design code calculations, and 20 times the performance of BlueGene/L (sited in 2005) on a weapons science materials calculation. The Sequoia platform and its implementation project are named after the California redwood trees that are the tallest and largest in the world.

In addition to the expected 2011 final system delivery, the Sequoia contract will provide a smaller but significant initial delivery platform (called Dawn, a fast-growing redwood) beginning in 2008 to permit needed scaling and code development to ensure effective use of the final Sequoia platform. This initial delivery Dawn system is expected to have 10–20 percent of the processor count of the 2011 system and will be used for several demanding near-term programmatic deliverables, in particular to support UQ and "knob" elimination.

Fundamental benefits of Sequoia are agile design and responsive certification infrastructure, increased accuracy in material property data, improved models for understood physical processes known to be important, meeting of programmatic requirements for uncovering missing physics, and improvement of the performance of complex models and algorithms in design codes. All are necessary to achieve predictive simulation in support of transformation, and all are aligned with requirements of the ASC Roadmap and the NNSA Predictive Capability Framework.

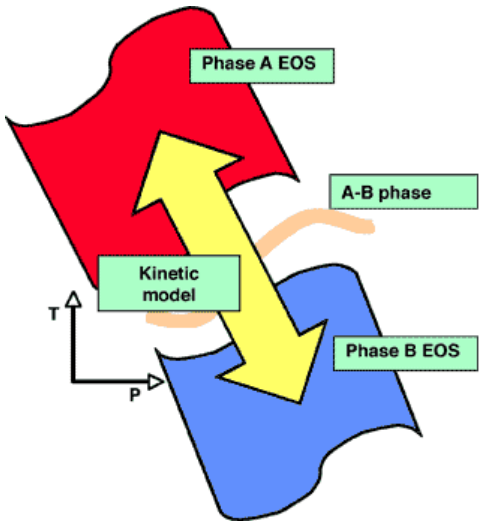
New Multiphase Plutonium Equation of State at LLNL Improves Current High Standard and Aids Stockpile Certification

Replacing an equation-of-state (EOS) high standard set in the 1990s for weapons simulation at Lawrence Livermore (LLNL), a new multiphase plutonium (Pu) EOS will allow weapons designers to elaborate important weapons-relevant physics beyond current capabilities. The new multiphase EOS moves simulations from a few-phase, single-table quantum-based representation to a more accurate many-phase, multi-table advanced quantum representation, while confirming and retaining the best and most trusted features of the current baseline EOS.

A complete tables package for LLNL's new multiphase EOS has been developed and implemented in LLNL hydrocodes, and application tests are in progress. General release of the tested tables is expected by October 1, 2007. As part of the NNSA Stockpile Stewardship Program, the EOS effort at LLNL focuses on understanding, elaborating, and tabulating the thermodynamic properties of stockpile materials for programmatic application. The need for an improved Pu EOS is driven by the primary performance requirements of quantifying margins and uncertainties (QMU). Towards this end, LLNL seeks to exploit the fact that the thermodynamic properties of a material are determined at the atomistic (nanometer)-length scale where rigorous quantum-mechanical methods apply. Using advanced electronic structure and atomistic simulation techniques implemented on ASC platforms, together with recent accurate static and dynamic experimental data, LLNL developed a next generation multiphase Pu EOS intended for stockpile certification and QMU, completing an LLNL 2007 ASC level 2 milestone.

EOS advancements made include:

- Extensive and successful application of advanced first-principles electronic structure and quantum-based many-body inter-atomic potential methods to the calculation of the high-pressure phase diagram and the required cold, ion-thermal and electron-thermal EOS components of each individual phase. In addition, generalization and extension of these methods to the low-density phases of Pu capture important and strongly correlated behavior among f electrons.
- Validation of the low-temperature EOS by diamond-anvil-cell synchrotron x-ray data from the Advanced Photon Source at Argonne National Laboratory and of the high-temperature EOS from JASPER shock data taken at the Nevada Test Site.
- Incorporation of both well-known phases and recently discovered new phases and phase lines into the multiphase EOS. Certain long-standing issues and uncertainties concerning the Pu phase diagram have yielded to accurate diamond-anvil-cell measurements, while theory has predicted some new and unexpected behavior at high pressure.
- Implementation and testing of a unique multi-table EOS framework within the LLNL hydrodynamic simulation codes ("hydrocodes") that will permit an optional treatment of phase kinetics, that is, nonequilibrium, time-dependent transitions between phases. The inherently modular nature of this framework will also allow easier future updates and repairs of the EOS.

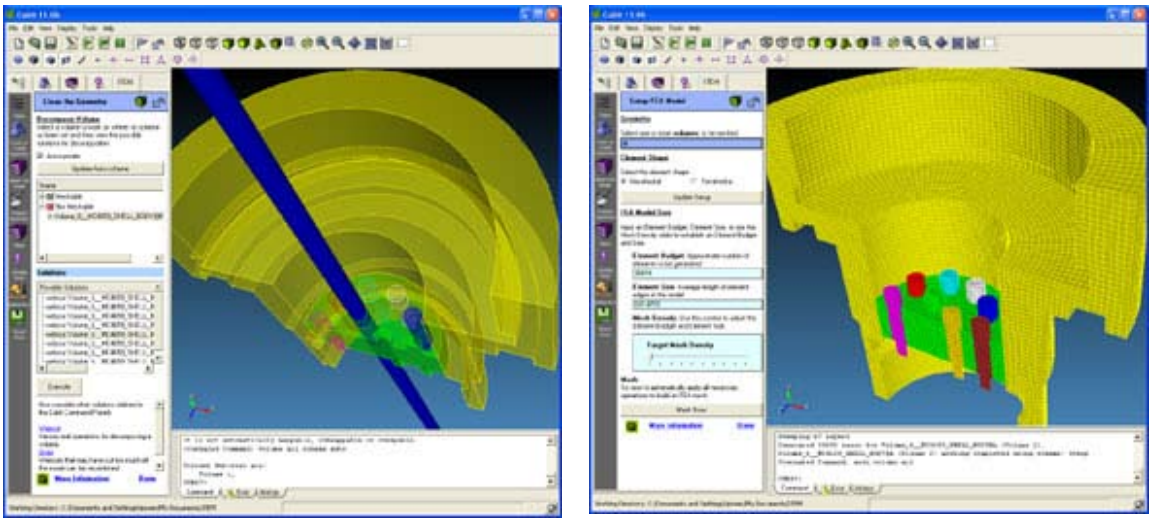


SCHEMATIC REPRESENTATION OF A PHASE TRANSITION IN THE NEW MULTIPHASE, MULTI-TABLE PLUTONIUM EQUATION OF STATE.

CUBIT Advances Automation of Geometry Preparation and Meshing

CUBIT is a toolkit for robust and unattended generation of two- and three-dimensional finite element meshes (grid).

To address an ASC level 2 milestone, Sandia's CUBIT team has developed a new environment for guiding analysts through the process of generating a hexahedral or tetrahedral mesh for simulation. This new environment is called the Immersive Topology Engine for Meshing (ITEM) and is built on the existing CUBIT Geometry and Meshing Toolkit. New geometric reasoning algorithms have been developed that can detect potential problems in a CAD model and provide a list of suggested solutions. This is offered in a wizard-like environment where the user may systematically step through the geometry preparation and meshing process and run a series of diagnostic tests. The user is then presented with a list of solutions to specific geometric problems that can be easily previewed and performed at will. With phase 1 of ITEM now complete, this tool can now generate diagnostics and solutions for a range of geometric problems, including resolving small features, detecting and fixing imprint/merge problems, and detecting potential decomposition options for hexahedral sweeping. Scheduled to be completed in August 2007, this new tool promises to dramatically improve the productivity of analysts who currently must spend considerable time developing meshes for simulation.



An example of ITEM used to mesh a CAD model representing a weapon component. Left: ITEM detects and previews an option for decomposing the model for hexahedral mesh. Right: The final hexahedral mesh after using ITEM to help prepare the CAD model.

For further information contact Steve Owen, sjowen@sandia.gov

ASC Purple Capability System Completes First Cycle Under New Usage Governance Model

Because a capability class system is similar in value and uniqueness to a large experimental facility, a governance model was set up in 2005 to allocate cycles on ASC Purple as an ongoing series of six-month campaigns. ASC Purple completed its first six months operating as a national user facility on April 16, 2007. In this first effort, ASC Purple supported three tier-one Capability Computing Campaigns (CCCs). Each campaign received significant cycles on the Purple system to meet important ASC programmatic deliverables. Technical leads for these CCCs will soon be reporting to ASC headquarters on accomplishments and lessons learned. In addition, the process to award the second round of CCC allocations on Purple is now under way. The Campaign 2 call has resulted in 20 proposals from across the three defense laboratories; the proposals are now being prioritized. ASC hopes to begin Campaign 2 on May 29, 2007.

The ASC Purple capability system at Lawrence Livermore is the only ASC system to be managed under this governance model. Major ASC Purple programmatic computing efforts are organized as computing

work packages or CCCs and are reviewed and prioritized for relevance, importance, and technical rationale. Each proposed CCC consists of at least one major calculation needing a significant proportion of an ASC capability system, together with related supporting jobs of smaller sizes. The objectives of the governance model are twofold: to ensure capability system resources were allocated on a priority-driven basis according to program requirements and to use ASC capability systems to run the large capability jobs for which the systems were designed and procured.

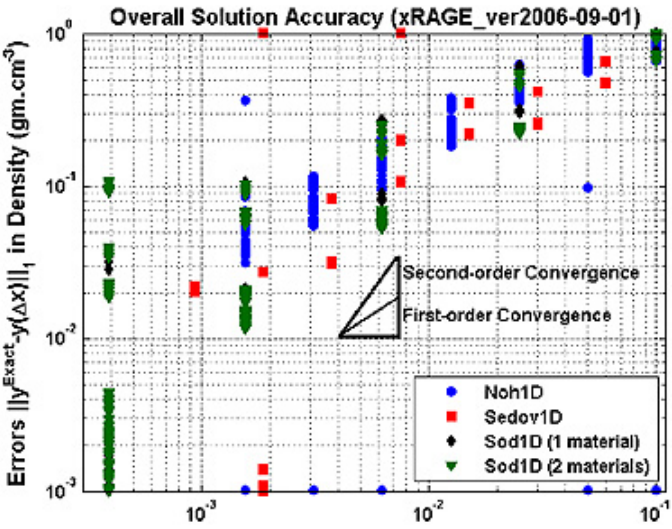
Roadrunner Project Completes Major Milestone

The Roadrunner Project completed a major milestone in December 2006 with the Final Acceptance of the Roadrunner Base System. The Roadrunner Base System is 14 connected units (~71 teraFLOPS) for the classified computing environment and 2 connected units (~10 teraFLOPS) for the unclassified computing environment. The completion of the acceptance testing was a joint effort between IBM and Los Alamos staff. The Roadrunner Base System is intended to provide a large "capacity-mode" computing resource for LANL weapons simulations. With the completion of this milestone, on schedule, the system is now ready for additional systems integration and application readiness work in preparation for limited production in spring of 2007.

Large Dataset Generated for the Verification of an ASC Code

During March 2007 Marine Marcilhac, Division X-1 postdoc at Los Alamos (LANL), and François Hemez, X-1 technical staff member, completed 12,256 simulation runs with an ASC code to quantify numerical uncertainty. Part of the Code Verification project, headed at LANL by X-1's Jerry Brock, the project's goals are to develop methodologies for code and solution verification, assess time-to-solution, and quantify solution uncertainty in support of programmatic deliverables.

The investigated algorithm is a finite-volume Godunov solver for the compressible equations of hydrodynamics in Eulerian frame-of-reference, developed by the Crestone Code Project at LANL. Six test problems were analyzed (Noh, Sedov, Woodward-Corolla interactive waves, and three variants of the Sod shock tube). Although this demonstration is currently restricted to 1D geometry, the dataset includes smooth and shocked solutions, convergent and divergent flows, and various patterns of wave interaction. A computer experiment was designed to vary the grid refinement, Courant condition, time-step controls, and four other options of the numerical method. Depending on settings of the calculation and numerical method, running times for analysis of each test problem varied between 10 seconds and 8 hours, using four processors of the QSC Platform at LANL. Generating such a large dataset was a significant effort that tested the ability of a toolbox developed to generate designs-of-computer-experiments; write, organize, and submit multiple input decks for parametric study; upload and post-process the results; perform effect screening and analysis-of-variance; and analyze the solution quality as a function of grid refinement.



The figure represents the L1 norms of the differences between exact and discrete solutions as a function of grid sizes used. The solution errors are shown for the density field of four test problems representing 11,552 runs. The figure illustrates two main findings of the study: (1) the numerical method is first-order accurate, as expected when discontinuous solutions, such as those of the four test problems shown, are computed. (2) solution accuracy is sensitive to the choice of numerical options used in the calculation. The figure also indicates that greater accuracy tends to be achieved at the cost of increased sensitivity to the method of performing the simulation.

W76-1 Qualification Simulations Completed with Sandia's Engineering Codes on Red Storm

Intense computational efforts with Sandia's engineering codes were completed on Red Storm to support the qualification of the arming, fuzing and firing (AF&F) system for the W76-1 Life Extension Program. This effort included several diverse sets of high-fidelity simulations in which uncertainties were quantified in each application. The applications included the behavior of the AF&F under abnormal drop conditions, system behavior under normal thermal environments, radiation transport to the AF&F under hostile radiation environments, and the structural dynamics response of the AF&F to hostile environments. These applications required the use of the explicit dynamics, thermal, and structural dynamics capabilities in SIERRA Mechanics and the radiation transport capabilities in RAMSES. SIERRA Mechanics and RAMSES are two of Sandia's engineering codes that provide mechanical/thermal/fluid and radiation/electrical capabilities, respectively. The calculations required 35% of Red Storm for more than three months ending in January 2007.

Tri-lab Linux Capacity Cluster Procurement Will Support Stockpile Stewardship Program

The Tri-laboratory Linux Capacity Cluster 2007 (TLCC07) procurement draft request for proposal, released in April 2007, sets the stage to supply hundreds of teraFLOPS of production capacity simulation cycles for the nation's three defense laboratories: Lawrence Livermore, Los Alamos, and Sandia. The large-scale capacity computing platforms will be used to support the Stockpile Stewardship Program mission of the NNSA through the ASC Program. The TLCC07 clusters will be delivered to the three laboratories in stages, with the first scalable units being delivered in the fourth quarter of 2007.

The draft TLCC07 request for proposal is now available. Currently, the Livermore Site Office and the DOE contracts department are reviewing the proposal package. Once approved, the final request for proposal package will be released to industry.

The TLCC07 procurement, led by Lawrence Livermore, will:

- Provide a common capacity computing platform and software environment for clusters across the three laboratories. This environment will reduce the complexity of cluster deployment and support, thus making it easier for users to run applications at any site while reducing the amount of computing environments needing code development support.
- Build clusters by purchasing a set of nodes in which all cluster components are contained, also known as a scalable unit. The scalable unit concept allows vendors to apply the might of volume manufacturing practices by building up to 20 to 30 scalable units while retaining the ability to deploy clusters consisting of 2, 4, 6, or 8 scalable units at the different sites.
- Significantly lower overall cluster total cost of ownership for the ASC Program and NNSA.

Red Storm Upgrade Evaluation Receives ISC Best Paper Award

Sandia researchers were awarded one of two Best Paper awards at the 2007 International Supercomputing Conference (ISC). The paper, entitled "An Evaluation of the Impacts of Network Bandwidth and Dual-Core Processors on Scalability," analyzes the impact of the processor and network upgrade of the Red Storm system at Sandia on ASC applications. Authors are Ron Brightwell, Keith Underwood, and Courtenay Vaughan.

The paper describes the hardware and software upgrade of the Red Storm system and analyzes application scaling and performance, comparing single-core and dual-core processors. Results showed that adding a second core provides from 20% to 50% performance boost on a fixed problem size per sock-

et basis. Results also indicate that application scalability is impacted relatively little by the upgrade. Most degradation in parallel efficiency is directly attributable to contention for resources caused by having two cores in one socket; however, with the doubling in message passing interface tasks that is typical of using dual-core processors, it is possible to see scaling effects detrimental to overall performance when running at the largest scale.

ISC is the leading Supercomputing Conference and Exhibition in Europe. Each of the two Best Paper awardees for ISC are given a EUR 5000 prize sponsored by Microsoft. The award will be presented June 26, 2007, in Dresden, Germany.

See more info at http://www.supercomp.de/isc2007

Lawrence Livermore Researchers Win Best Paper Award at Computing Symposium

Lawrence Livermore researchers Bronis de Supinski and Martin Schulz, along with North Carolina State University faculty member Frank Mueller and his student Mike Noeth, won the best paper award in the software track for the 2007 International Parallel and Distributed Processing Symposium, held March 26 to 29 in Long Beach, CA.

Their paper, "Scalable Compression and Replay of Communication Traces in Massively Parallel Environments," addresses the issue of significantly growing processor counts in high-end computer systems in terms of message passing interface (MPI) performance and current tool paradigms. For example, message passing trace mechanisms typically result in file sizes proportional to the number of processors and to the job's execution time. Work highlighted in the paper presents new mechanisms for tracing MPI events, resulting in near-constant trace file sizes as problem size and/or processor counts are increased. Further, the compression mechanism automatically detects communication patterns that may facilitate the determination of good task mappings on architectures that provide significant rewards for recognizing a communication locality such as that of the ASC Program's BlueGene/L computer. Further extensions to this work promise to detect anomalous MPI performance events in the traces automatically.

High-end computer systems are growing significantly in total processor count. BlueGene/L has over 131,000 processor cores. Two-hundred-and-twenty-eight systems on the recent Top500 list (45.6 percent) had over 1,024 processors, and 18 systems had over 8,192 processors.

ASC Salutes—John Turner

John Turner joined Los Alamos (LANL) in 1990, in the area of Nuclear Reactor Safety and Analysis, after completing his Ph.D. in Nuclear Engineering from North Carolina State University. In 1992, he moved to X-Division to work on deterministic radiation transport in the group that would later become CCS-4. During this time, he also contributed, as a founding team member, to the casting simulation effort being initiated in the Fluid Dynamics Group, T-3. This project became Telluride, and is increasingly contributing to the improvement of manufacturing processes at LANL and elsewhere. John departed LANL, in 1997, for a stint at Blue Sky Studios, a computer animation company outside New York City.

At Blue Sky, John contributed algorithmic and performance improvements to the proprietary ray-tracing renderer used to generate all the company's images, and developed other tools such as a 2D incompressible flow code used to simulate lava flow in the Academy Award-nominated feature film, *Ice-Age*. In addition to credits on *Ice Age*, he is also credited on the Academy Award-winning short animated film *Bunny*.

Returning to LANL and the Telluride project in 2001, John progressed to group leader of CCS-2 and an active involvement in modeling and simulation for the resurgence of nuclear power within the Global Nuclear Energy

Partnership (GNEP). He serves as principal investigator on the Advanced Architecture LDRD-DR, which has developed tools and applications for emerging hybrid and heterogeneous computing architectures such as the use of video cards, Graphical Processing Units (GPUs), and high-performance co-processors. The diversity of John's experience is well-attuned to the upcoming Roadrunner supercomputer, which will use the Cell Broadband Engine—the Playstation 3 video game console processor—in conjunction with an Opteron-based Linux cluster to reach the 1 PetaFLOP performance goal. In this context, John is leading the Advanced Algorithms and Assessment team, tasked with ensuring that Roadrunner achieves high performance not just on synthetic benchmarks but on applications of scientific interest to LANL. Given John's experience with hybrid architectures and the diversity of his code-development successes, he is expected to be an invaluable asset in the evolution of Roadrunner and its potential impact on the ASC Program.

Comings and Goings

Karen Pao is the new V&V Program Manager at HQ. She comes from Los Alamos.

Tom Bickel is the new ASC Executive at Sandia. He replaces Art Hale, who left the ASC program to become the new Chief Information Officer at Sandia.

Effective March 30, **James Peery** left his position as LANL's Hydrodynamic Experiment (HX) Division Leader to accept a position at Sandia National Laboratories as Center Director for Computation, Computers, Information and Mathematics. Weapons Physics will miss James's leadership. Associate Director Charles F. McMillan asked Peery's Deputy Division Leader, Rollin Whitman, to serve as Acting Division Leader for HX.

ASC Web Site

http://www.sandia.gov/NNSA/ASC/

Newsletter Points of Contact

Send submittals to:
Vin Lopresti—Los Alamos National Laboratory vcl@lanl.gov
Andrea Baron—Lawrence Livermore National Laboratory baron1@llnl.gov
Reeta Garber—Sandia National Laboratories ragarbe@sandia.gov

Who's Who

ASC Program Managers—Headquarters

Director, Office of Advanced Simulation and Computing, NA-114
Dimitri Kusnezov—Dimitri.Kusnezov@nnsa.doe.gov

Ken Alvin—kfalvin@sandia.gov
April Commodore—april.commodore@nnsa.doe.gov
Njema Frazier—njema.frazier@nnsa.doe.gov
Thuc Hoang—thuc.hoang@nnsa.doe.gov
Sander Lee—sander.lee@nnsa.doe.gov
Ed Lewis—edgar.lewis@nnsa.doe.gov
Bob Meisner—bob.meisner@nnsa.doe.gov
Denise Peoples—denise.peoples@nnsa.doe.gov
Erich Rummel—erich.rummel@nnsa.doe.gov
Karen Pao—kip@lanl.gov

ASC Program Managers—Labs

Los Alamos National Laboratory
John Hopson—jhopson@lanl.gov
Cheryl Wampler—clw@lanl.gov
Ralph Nelson, Deputy Program Director (acting)—ran@lanl.gov

Lawrence Livermore National Laboratory
Michel McCoy—mccoy2@llnl.gov
Lynn Kissel, Deputy Program Manager—kissel1@llnl.gov

Sandia National Laboratories
Tom Bickel—tbickel@sandia.gov
Marty Pilch, QMU and Management Support—mpilch@sandia.gov
Paul Yarrington, Weapon Simulation & Computing—pyarrin@sandia.gov

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